Density Matrices. 6/25/2020

$|\psi_i\rangle = \begin{bmatrix} \vdots \end{bmatrix}$

- $|\psi_i\rangle$: a particular state
  - p_i : corresponding probability

Notice: we assume that $|\psi_i\rangle$ is normalized, so $\langle\psi_i||\psi_i\rangle = 1$.

- for observable a, the mean value is:

$$\langle A\rangle = \sum_{i=1}^{N} p_i \boxed{\langle\psi_i| A |\psi_i\rangle}$$

→ it's a scalar. (Quadratic forms.)

"weights"

$\langle\psi_i|$: conjagate transpose of $|\psi_i\rangle$

- Then, density matrix is defined as:

$$\rho = \sum_{i=1}^{N} p_i \underbrace{|\psi_i\rangle\langle\psi_i|}_{\text{a rank-one matrix}}$$

xx^* → $\begin{bmatrix} \vdots \end{bmatrix}\begin{bmatrix} \cdots \end{bmatrix}$ ⇒ rank-1

↝ a linear combination of composite states.

- Can rewrite: $\langle A\rangle = \mathrm{tr}(\rho A)$. ←

ψ_i : eigenvector.

→ Look at it in a "math" way:

↳ if we write it as: x ↙ eigenvector, then $\langle\psi_i| A |\psi_i\rangle \Leftrightarrow x^*Ax$

⇒ $\lambda x = Ax$, so $x^*Ax = x^*\lambda x = \lambda\, x^*x \overset{1}{} = \lambda$

⇒ so, we basically sum up the eigenvalues.

⇒ $\sum_i \lambda_i$ = trace. ↙ sum of the diagonal entries.

→ Look at it in a "physics" way:

A : physics operator
ρ : density
} ⇒ ρA : mean

Density Matrices

Hermitian: eigenvectors can be taken to be a orthonoral set.

- **Example** : 2.4.

Pure state : $\rho = \langle\psi||\psi\rangle$

$$\langle A\rangle = tr(\rho A) = \sum_i \underbrace{\langle\psi_i|\underbrace{\psi\rangle\langle\psi}_{\rho}|A|\psi_i\rangle}_{i^{th}\text{ diagonal entry}} = \sum_i \overbrace{\langle\psi|A|\psi_i\rangle}^{\text{scalar}}\overbrace{\langle\psi_i|\psi\rangle}$$

$$= \langle\psi|A\underbrace{\sum_i|\psi_i\rangle\langle\psi_i|}_{\text{Identity.}}\psi\rangle$$

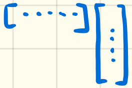
$$= \langle\psi|A|\psi\rangle.$$

- A general density matrix is a convex combination of pure state.

- Convex combination: a linear combination of points where all coefficients are non-negative and sum to 1.

Positive Definite, Positive Semidefinite, etc.

Recall: $|\psi\rangle$: similar to vectors



$\overset{x^*}{\langle\psi|}\overset{A}{A}\overset{x}{|\psi\rangle}$: similar to quadratic forms: x^*Ax

Positive Definite (PD): $Q(x) = x^*Ax > 0$ $\forall\ x \neq 0$

Pos. Semidefinite (PSD): $Q(x) = x^*Ax \geq 0$.

Note: PD: for Hermitian matrices.

Similarly: Negative Definite. (ND) $Q(x)$ → a function denpends on x.

↳ $x^*Ax < 0$

Neg. ~ Semidefinite (NSD) $x^*Ax \leq 0$

Also: Indefinite (ID).

What's x^*Ax ?

x^*Ax : Quadratic forms.

Maximizing ? $\begin{cases} x_1^* x_2 = 0 \\ x_1^* x_1 = 1. \end{cases}$

Suppose: $\underset{\underset{\text{Hermitian}}{\uparrow}}{\underline{A = A^*}}$, $\underset{n \times n}{\underline{A \in M_n}}$. → $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ eigvals

$\underline{x_1} \quad \underline{x_2} \quad \cdots \quad \underline{x_n}$ eigvec.

↳ For Hermitian Matrices, eigenvectors can always be taken as an orthonormal set. (so it's a basis for $\mathbb{R}^n / \mathbb{C}^n$)

Pick: arbitrary x,

$$\underline{x = \alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_n x_n}.$$

$|\alpha_i|^2 = \alpha_i \overline{\alpha_i}$ ↑

$$x^* x = \Sigma(\overline{\alpha}_i x_i^*)(\alpha_j x_j) = \Sigma |\alpha_i|^2.$$

$i \neq j$, $x_i^* x_j = 0$.

$$x^*Ax = x^* \underline{\Sigma \alpha_i \lambda_i x_i} = \underline{\Sigma\, \overline{\alpha}_i \alpha_i \lambda_i \overset{=1}{\boxed{x_i^* x_i}}} = \boxed{\Sigma |\alpha_i|^2 \lambda_i}.$$

↑ put A back: $A(\alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_n x_n)$.

$= \Sigma \alpha_i A x_i$

$= \Sigma \alpha_i \lambda x_i$

weighted average of λ_i.

So, for $\underline{Q(x) > 0}$ $\forall$ $\underline{x \neq 0}$,

need: $\underline{\lambda_i > 0}$, $\forall i$.

Similarly ⇒

PSD : $Q(x) \geq 0$ $\quad \lambda_i \geq 0$ $\quad \forall i$

ND : $Q(x) < 0$ $\quad \lambda_i < 0$

NSD : $Q(x) \leq 0$ $\quad \lambda_i \leq 0$

ID : some $\lambda_i > 0$, some $\lambda_j < 0$.

Spectral Decomposition :

$$\underline{x^*Ax} = |\underset{\Delta}{\alpha_1}|^2 \underset{\uparrow}{\lambda_1} + |\underset{\Delta}{\alpha_2}|^2 \underset{\uparrow}{\lambda_2} + \cdots + |\underset{\Delta}{\alpha_n}|^2 \underset{\uparrow}{\lambda_n}$$

Max & Min of x^*Ax

$Q(x) = x^*Ax = \Sigma|\alpha_i|\lambda_i.$

$x = \alpha_1 x_1 + \alpha_2 x_2 + \cdots + \alpha_n x_n$

$$\max_{\underbrace{x^*x=1}_{\text{realized by:}}} x^*Ax = \lambda_n \quad \text{(put all weights on } \lambda_n.)$$

realized by: $x = x_n.$

$\alpha_n = 1.$

$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n.$

↑ max.

$$\min_{x^*x=1} x^*Ax = \lambda_1 \quad \text{(put all weights on } \lambda_1.)$$

realized by taking $x = x_1$

$$\min_{\substack{x^*x=1 \\ \boxed{x \perp x_1}}} x^*Ax = ? \quad \lambda_2$$

realized by taking $x = x_2$

PSD

$Q(x) \geqslant 0$

$\lambda_1 \geqslant 0$

$\min x^*Ax \geqslant 0$

... So What ? ⇒ Hermitian matrices : physics observable.

In mixed state,

- Density matrices are positive semidefinite (PSD). $x^*Ax \geqslant 0$ $\langle \psi_i | A | \psi_i \rangle \geqslant 0.$

- If ρ is separable, then the partial transpose are PSD.